Carlo Carlo

Access DB# 89405

# SEARCH REQUEST FORM

Scientific and Technical Information Center

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Requester's Full Name: Kahs	ay MbK	Examiner #	:78271 D	ate: Mar. 19, 2003
Art Unit: 1624 Phone	Number 30% - 9	711 Serial N	Number: //9/°	184273
Mail Box and Bldg/Room Location	on: 4E-18	_ Results Format Pre	eferred (circle): P	APER DISK E-MAIL
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Please provide a detailed statement of th	e search topic, and de	escribe as specifically as	possible the subject	matter to be searched.
Include the elected species or structures, utility of the invention. Define any term	is that may have a spe	ecial meaning. Give exa	numbers, and comb mples or relevant cite	ations, authors, etc., if
known. Please attach a copy of the cover	r sheet, pertinent clair	ms, and abstract.		
Title of Invention:				
Inventors (please provide full names):				
provide ran number).				
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Earliest Priority Filing Date:	,		~/\ \ \ \ \	lease see attache
*For Sequence Searches Only* Please incl appropriate serial number.			ional, or issued patent	numbers) along with the
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PTO-1500 (1-2000)

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FILE COVERS 1907 - 20 Mar 2003 VOL 138 ISS 12 FILE LAST UPDATED: 19 Mar 2003 (20030319/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

VAR G1=2/3/4/5 REP G2=(0-6) C VAR G3=71/SO2 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L5 11004 SEA FILE=REGISTRY SSS FUL L3

L14 STR

VAR G1=2/3/4/5
REP G2=(0-6) C
VAR G3=71/SO2
VAR G4=C/N
VAR G5=71/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L15 80 SEA FILE=REGISTRY SUB=L5 SSS FUL L14
L16 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L15

=> =>

=> d ibib abs hitstr 116 1

L16 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2001:636067 HCAPLUS

DOCUMENT NUMBER:

135:195577

TITLE:

Preparation of arylpiperazines and arylpiperidines as

metalloproteinase inhibiting agents

INVENTOR(S):

Barlaam, Bernard Christophe; Dowell, Robert Ian; Newcombe, Nicholas John; Tucker, Howard; Waterson,

David

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATEN	NT NO	ο.		KI	ND :	DATE			A	PPLI	CATI	N NC	ο.	DATE			
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WO 20	00106	6275	51	A.	1 :	2001	0830		M	O 20	01-G	В616		2001	0215		
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	C	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
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	I	ĹŪ,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,	RO,	RU,
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1261595 20021204 A1 EP 2001-905883 20010215

AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

NO 2002003951 20020820 NO 2002-3951 20020820 PRIORITY APPLN. INFO.: EP 2000-400469 Α 20000221 WO 2001-GB616 20010215

OTHER SOURCE(S): MARPAT 135:195577

GT

$$\begin{array}{c|c} B & & & \\ & X & & \\ & N & \\ & S_2 & & \\ & O & & N & \\ \end{array}$$

AΒ The title compds. [I; B = (un) substituted Ph, 2-pyridyl, 2-pyridyloxy, 4-pyrimidinyl; X = C, N; R1 = (trimethyl-1-hydantoin)alkyl,(un) substituted Ph, phenylalkyl, etc.], useful as metalloproteinase inhibitors, esp. as inhibitors of MMP 13, were prepd. E.g., a 5-step synthesis of I [B = 4-FC6H4; X = CH; R1 = CH2Ph] was given.

357187-74-7P 357187-78-1P 357187-79-2P ΙT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpiperazines and arylpiperidines as metalloproteinase inhibiting agents)

RN 357187-74-7 HCAPLUS

CN Benzeneacetamide, .alpha.-[[[4-(5-chloro-2-pyridinyl)-1piperazinyl]sulfonyl]methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 357187-78-1 HCAPLUS /

CN Benzeneacetamide, 4-chloro-.alpha.-[[[4-(5-chloro-2-pyridinyl)-1piperazinyl]sulfonyl]methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ C-NH-OH \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\$$

RN 357187-79-2 HCAPLUS

CN Benzeneacetamide, 3,4-dichloro-.alpha.-[[[4-(5-chloro-2-pyridinyl)-1-piperazinyl]sulfonyl]methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

IT 357187-91-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of arylpiperazines and arylpiperidines as metalloproteinase inhibiting agents)

RN 357187-91-8 HCAPLUS

CN Benzeneacetic acid, .alpha.-[[[4-(5-chloro-2-pyridinyl)-1-piperazinyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

### => d ibib abs hitstr 116 2

L16 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS 2001:636059 HCAPLUS ACCESSION NUMBER:

135:211053 DOCUMENT NUMBER:

Preparation of N-[2-(piperidino- or TITLE:

piperazino) sulfonylethyl] - N-hydroxyformamides as

inhibitors of metalloproteinases

Barlaam, Bernard Christophe; Dowell, Robert Ian; INVENTOR(S):

Finlay, Maurice Raymond Verschoyle; Newcombe, Nicholas

John; Tucker, Howard; Waterson, David

Astrazeneca AB, Swed.; Astrazeneca UK Limited PATENT ASSIGNEE(S):

PCT Int. Appl., 69 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	TENT	NO.		KI	ND	DATE			A	PPLI	CATIO	ои ис	ο.	DATE			
WO	2001	0627	42	 A	 1	2001	0830		− W	0 20	01-GI	 В624		2001	0215		
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EP	BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1261590 A1 20021204 EP 2001-905885 20010215																
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IIS	2002											8868	7	2001	0221		
	2002													2002			
PRIORIT														2000			
11(101(11			11110	• •													
OTHER S	WO 2001-GB624 W 20010215 OTHER SOURCE(S): MARPAT 135:211053																

GΙ

$$\begin{array}{c|c} B & & \\ X & & \\ N & & \\ S_{02} & & \\ & & \\ HO & & CHO & I \end{array}$$

The title compds. [I; B = (un)substituted Ph, 2-pyridyl, 2-pyridyloxy, AB 4-pyrimidinyl; X = CH, N; R1 = phenylalkyl, pyridylalkyl, pyrimidinylalkyl, etc.], useful as metalloproteinase inhibitors, esp. as inhibitors of MMP 13 (no data given), were prepd. E.g., a 4-step synthesis of I [B = 4-BrC6H4; X = N; R1 = 3-(pyrimidin-2-yl)propyl] was given. The compds. I are effective at 0.5-30 mg/kg/day.

357645-52-4P 357645-55-7P 357645-57-9P ΙT 357645-58-0P 357646-20-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of N-[2-(piperidino- or piperazino)sulfonylethyl]-N-hydroxyformamides as inhibitors of metalloproteinases)

RN 357645-52-4 HCAPLUS

CN

Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-[3-(phenylmethoxy)phenyl]ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 357645-55-7 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-[3-(trifluoromethyl)phenyl]ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 357645-57-9 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-[4-(trifluoromethyl)phenyl]ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 357645-58-0 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-thienyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN

357646-20-9 HCAPLUS
Piperazine, 1-[[2-(4-chlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME) CN

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

### hitstr 116

L16 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS 2000:161258 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:207849

Preparation of arylpiperazines as metalloproteinase TITLE:

inhibiting agents (MMP)

INVENTOR(S): Barlaam, Bernard Christophe; Newcombe, Nicholas John;

Tucker, Howard; Waterson, David

PATENT ASSIGNEE(S): Zeneca Limited, UK; Zeneca-Pharma Sa

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P.	ATE	ENT 1	NO.		KIND DATE APPLICATI					CATI	ои ис	ο.	DATE						
W	0 2	20000	0124	78	Α	1	2000	0309			WO	199	99-G	B280	1	1999	0825		
		W:	ΑE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB	3,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
																HR,			
			IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ	,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,
			MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL	٠,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,
																ZW,			
			KG,	KΖ,	MD,	RU,	ТJ,	TM											
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ	ζ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,
			ES,	FI,	FR,	GB,	GR,	ΙE,	ΙT,	LU	J, :	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,
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										EΡ	19	99-	4013	51	Α	1999	0604		
											19	99-0	GB28	01	W	1999	0825		
OTHER GI	SOU	JRCE	(S):			MAR	PAT	132:	2078	49									

Page 8

AB The title compds. [I; B = monocyclic or bicyclic alkyl, aryl, etc.; R3 = H, halo, NO2. etc.; n = 1-3; P = (CH2)n (wherein n = 0-2), alkene, alkyne, etc.; A = (un)substituted 5-7 membered aliph. ring; X1, X2 = N, C, where a ring substituent on ring A is a oxo group that is preferably adjacent a ring N atom; Y = SO2, CO; Z = CONHOH, Y = CO and Q = CR6R7, CR6R7CH2, NR6, NR6CH2 (wherein R6 = H, alkyl, aralkyl, etc.; R7 = H, alkyl; R7 together with R6 forms a carbocyclic or heterocyclic spiro 5-7 membered ring, the latter contg. at least one heteroatom selected from N, O, S); Z = CONHOH, Y = SO2 and Q = CR6R7, CR6R7CH2; Z = N(OH)CHO and Q = CHR6, CHR6CH2, NR6CH2; R1 = H, alkyl, cycloalkyl, etc.; R2 = H, alkyl, aryl, etc.], useful as metalloproteinase inhibitors (no data), esp. as inhibitors of MMP 13, in treating arthritis and atherosclerosis, were prepd. E.g., a multi-step synthesis of the title piperazine II was given. Compds. I are effective at 0.5-30 mg/kg/day.

260438-29-7P 260438-30-0P 260438-32-2P 260438-37-7P 260439-09-6P 260439-10-9P 260439-31-4P 260439-32-5P 260440-19-5P 260440-23-1P 260440-57-1P 260440-84-4P

260440-89-9P 260440-99-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpiperazines as metalloproteinase inhibiting agents  $(\mathsf{MMP})$ )

RN 260438-29-7 HCAPLUS

CN Piperazine, 1-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfony l]-4-[5-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)

RN 260438-30-0 HCAPLUS

CN Piperazine, 1-[[2-(4-bromo-2-thienyl)-2-(formylhydroxyamino)ethyl]sulfonyl ]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 260438-32-2 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260438-37-7 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(2-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260439-09-6 HCAPLUS

CN Piperazine, 1-(6-chloro-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260439-10-9 HCAPLUS

CN Piperazine, 1-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-4-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260439-11-0 HCAPLUS

CN Piperazine, 1-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfony l]-4-(4-methyl-2-quinolinyl)- (9CI) (CA INDEX NAME)

RN 260439-17-6 HCAPLUS

CN Piperazine, 1-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfony l]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} OH & C1 \\ OOHC-N \\ \parallel \\ S-CH_2-CH \end{array}$$

RN 260439-18-7 HCAPLUS

CN Piperazine, 1-[[2-(formylhydroxyamino)-2-[4-(trifluoromethyl)phenyl]ethyl] sulfonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 260439-31-4 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-cyclopentyl-2-(formylhydroxyamino)ethyl]sulfonyl]-(9CI) (CA INDEX NAME)

RN 260439-32-5 HCAPLUS

CN Piperazine, 1-(5-cyano-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260439-80-3 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[(2S)-2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 260440-05-9 HCAPLUS

CN Piperazine, 1-[[2-(formylhydroxyamino)-2-phenylethyl]sulfonyl]-4-(5-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 260440-10-6 HCAPLUS

CN Piperazine, 1-[[2-(formylhydroxyamino)-2-phenylethyl]sulfonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 260440-19-5 HCAPLUS

CN Piperazine, 1-[[2-(formylhydroxyamino)-2-phenylethyl]sulfonyl]-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 260440-23-1 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[4-[[2-(formylhydroxyamino)-2-phenylethyl]sulfonyl]-1-piperazinyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 260440-57-1 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260440-84-4 HCAPLUS

CN Piperazine, 1-(5-cyano-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260440-89-9 HCAPLUS

CN Piperazine, 1-(5-bromo-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 260440-99-1 HCAPLUS

CN Piperazine, 1-[[2-(5-bromo-3-pyridinyl)-2-(formylhydroxyamino)ethyl]sulfon yl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)

IT 260441-75-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of arylpiperazines as metalloproteinase inhibiting agents
 (MMP))

RN 260441-75-6 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-(hydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

IT 260441-62-1P 260441-63-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of arylpiperazines as metalloproteinase inhibiting agents
(MMP))

RN 260441-62-1

CN Piperazine, 1-[[(2S)-2-[[(4.xi.)-2,3:5,6-bis-O-(1-methylethylidene)-D-ribohexofuranosyl]hydroxyamino]-2-(3-pyridinyl)ethyl]sulfonyl]-4-(5-chloro-2pyridinyl) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

260441-63-2 HCAPLUS Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[(2S)-2-(hydroxyamino)-2-(3-CN pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

#### => d ibib abs hitstr 116 4

AUTHOR(S):

L16 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS

1996:6879 ACCESSION NUMBER: HCAPLUS

DOCUMENT NUMBER: 124:176036

Design, Synthesis, and Structure-Activity Relationship TITLE:

Studies of Novel 1-[(1-Acyl-4-piperidinyl)methyl]-1H-2methylimidazo[4,5-c]pyridine Derivatives as Potent, Orally Active Platelet-Activating Factor Antagonists Carceller, Elena; Merlos, Manuel; Giral, Marta; Balsa,

Dolors; Garcia-Rafanell, Julian; Forn, Javier

CORPORATE SOURCE: Research Center, J. Uriach Cia. S.A., Barcelona,

08026, Spain

SOURCE: Journal of Medicinal Chemistry (1996), 39(2), 487-93

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Replacement of the polar head of the previously reported series of 1-acyl-4-[(2-methyl-3-pyridyl)cyanomethyl]piperazines with a 2-methylimidazo[4,5-c]pyridine group led to the identification of a new series of 1-[(1-acyl-4-piperidyl)methyl]-1H-2-methylimidazo[4,5-c]pyridine derivs. as potent, orally active platelet-activating factor (PAF) antagonists. On the basis of the general structure-activity relationship trends found for the acyl substituent in our earlier series, five groups of compds. were tested, i.e., diaryl- or alkylarylpropanoyl derivs., their 3-hydroxy-substituted analogs, and urea, carbamate and amino acid derivs. The optimal compd. UR-12670, bearing the 3,3-diphenylpropanoyl moiety, exhibited very high in vitro and in vivo potency (IC50 = 0.0076 .mu.M for the in vitro PAF-induced platelet aggregation assay, ID50 = 0.0086 mg/kg for the in vivo PAF-induced hypotension test in normotensive rats, and ID50 = 0.092 mg/kg po and 0.0008 mg/kg i.v. for the PAF-induced mortality test in mice). UR-12670 also showed long duration of activity. It gave 100% protection against PAF-induced mortality in mice 7 h after i.v. administration of a single dose of 1 mg/kg and also provided 100% inhibition of PAF-induced aggregation in dog whole blood 6 h after i.v. administration of the same dose. The lead structure UR-12670 was selected for in-depth pharmacol. evaluation.

ΙT 149692-09-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(structure activity relationship of (piperidinyl)methyl]imidazo[4,5c]pyridines as platelet activating factor antagonists)

RN 149692-09-1 HCAPLUS

Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-CN oxo-1-phenylpropyl]-, methyl ester (9CI) (CA INDEX NAME)

### => d ibib abs hitstr 116 5

L16 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1995:380148 HCAPLUS

DOCUMENT NUMBER: 122:160682

TITLE: Cyanomethylpyridine derivatives as PAF antagonists and

5-lipoxygenase inhibitors

INVENTOR(S): Carceller, Elena; Jimenez, Pere J.; Almansa, Carmen;

Bartoli, Javier

PATENT ASSIGNEE(S): J. Uriach y Cia. S.A., Spain

SOURCE:

Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent English

LANGUAGE: Enc FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		A1	19940928		19940323
	R: AT, BE, C	H, DE	, DK, ES, FR,	GB, GR, IE, IT, LI	, LU, MC, NL, PT, SE
	ES 2062943	A1	19941216		19930323
	ES 2062943	В1	19951116		
	CA 2118831	AA	19940924	CA 1994-2118831	19940311
	JP 07002841	A2	19950106	JP 1994-76436	19940323
	US 5420131	Α	19950530	US 1994-216583	19940323
PRIO	RITY APPLN. INFO.:			ES 1993-591	19930323
OTHER	R SOURCE(S):	MA	RPAT 122:160	682	
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The invention relates to cyanomethylpyridine derivs. I [Y = N or CH; R1 = AB F, C1; R2 = H or C1-4 alkyl; m = 0, 1 or 2; n = 0 or 1; p = 0 or 1; A = 0covalent bond, CONHCH(Ar), NHCH(Ar), SO2NHCH(Ar), NHCONHCH(Ar), or OCONHCH(Ar); and when p = 1, A can also = CH(Ar)NH; Ar = Ph or Ph substituted .gtoreq. 1 of halo, C1-4 alkyl, C1-4 alkoxy, or CF3]. compds. are platelet activating factor (PAF) antagonists and/or 5-lipoxygenase inhibitors, and are useful for treating a variety of diseases. For example, coupling of p-(2-quinolylmethoxy)phenylacetic acid with 1-(3-amino-3-phenylpropionyl)-4-[(2-methyl-3pyridyl)cyanomethyl]piperazine using DCC and 1-hydroxybenzotriazole in DMF gave 43% title compd. II, a preferred compd. The IC50 of II for inhibition of PAF-induced hypotension in normotensive rats was 0.036 mg/kg i.v. Twelve addnl. syntheses, addnl. biol. tests (inhibition of PAF-induced platelet aggregation, and inhibition of LTB4 prodn.), and 6 example formulations are given.

### IT 149691-83-8

RL: RCT (Reactant); RACT (Reactant or reagent)
 (amidation; prepn. of cyanomethylpyridine derivs. as PAF antagonists
 and 5-lipoxygenase inhibitors)

RN 149691-83-8 HCAPLUS

CN 1-Piperazineacetonitrile, 4-(3-amino-1-oxo-3-phenylpropyl)-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN \\ CH-N \\ Me \end{array}$$

$$\begin{array}{c|c} C-CH_2-CH-NH_2 \\ \parallel & \parallel \\ O \end{array}$$

# IT 161180-94-5P 161180-95-6P 161180-96-7P 161180-97-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of cyanomethylpyridine derivs. as PAF antagonists and 5-lipoxygenase inhibitors)

RN 161180-94-5 HCAPLUS

CN Benzeneacetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-4-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 161180-95-6 HCAPLUS

CN Benzeneacetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-B

N

RN 161180-96-7 HCAPLUS

CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-4-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

RN 161180-97-8 HCAPLUS

CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

### => d ibib abs hitstr 116 6

L16 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS 1994:106931 HCAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

120:106931

TITLE:

Synthesis and structure-activity relationships of 1-acyl-4-((2-methyl-3-pyridyl)cyanomethyl)piperazines

as PAF antagonists

AUTHOR(S):

Carceller, Elena; Merlos, Manuel; Giral, Marta; Almansa, Carmen; Bartroli, Javier; Garcia-Rafanell,

Julian; Forn, Javier

CORPORATE SOURCE:

Chem. Lab., J. Uriach e Cia.S.A., Barcelona, 08026,

Spain

SOURCE:

Journal of Medicinal Chemistry (1993), 36(20), 2984-97

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE:

LANGUAGE:

Journal

English

AB Title compds., e.g. I [R = Me, R1 = Ph2CHXCH2CO, PhCR2R3CH2CO, R4NHCHPhCO; X = CH2, CH2CH2, NH, NCHO, NAC, NSO2Me, O, S(O), SO2; R2 = OH, CO2Et, F, R3 = Ph, Me, CF3, 3-pyridyl; R4 = PhO2C, PhCH2O2C, MeO2C, EtO2C, Me2CHCH2O2C, Me3CO2C, H2NCO, pyrrolidinocarbonyl, Bz, 3-pyridylcarbonyl, 3-furylcarbonyl, 2-piperazinylcarbonyl, Ac, Me, PhSO2, MeSO2, H, Ph, PhCH2, 3-pyridylmethyl, H2C:CHCH2, HC.tplbond.CCH2], second generation (cyanomethyl)piperazines with increased oral activity were prepd. and evaluated in vitro in a platelet aggregation factor (PAF)-induced platelet aggregation assay and in vivo in a PAF-induced hypotension test in normotensive rats. Oral activity was ascertained through a PAF-induced mortality test in mice. I (R = Me) showed an order of magnitude or greater improvement in the oral ID50 test compared with I (R = H). different types of acyl substituents of similar potency emerge from this work: R1 = Ph2CHNHCH2CO, HOCR3PhCH2CO, and R4NHCHPhCH2CO. The most interesting compds., I (R = Me, R1 = Ph2CHNHCH2CO) (II) (UR-12460) and I (R = Me, R1 = MeO2CNHCHPhCH2CO) (UR-12519) (III) compare favorably with WEB-2086. II and III were also tested in active anaphylactic shock and endotoxin-induced mortality tests. On the basis of these data and addnl. pharmacol. development, II and III were selected for clin. testing.

ΙT 149692-22-8 149692-25-1

> RL: RCT (Reactant); RACT (Reactant or reagent) (platelet aggregation factor antagonistic activity of)

149692-22-8 HCAPLUS RN

CN 1-Piperazineacetonitrile, 4-[3-(methylamino)-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl) - (9CI) (CA INDEX NAME)

RN 149692-25-1 HCAPLUS

CN 1-Piperazineacetonitrile, 4-[3-[bis(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

IT 149691-77-0P 149691-84-9P 149691-85-0P 149691-86-1P 149692-10-4P 149692-11-5P 149692-12-6P 149692-13-7P 149692-14-8P 149692-15-9P 149692-16-0P 149692-17-1P 149692-18-2P 149692-20-6P 149692-21-7P 149692-24-0P 149692-26-2P 149692-27-3P 149692-28-4P 149692-29-5P 149692-30-8P 149692-31-9P 149692-41-1P 150812-47-8P 150812-48-9P 150812-49-0P 150812-50-3P 150812-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and platelet aggregation factor antagonistic activity of)

RN 149691-77-0 HCAPLUS

CN 1-Piperazinebutanoic acid, 4-[cyano(2-methyl-3-pyridinyl)methyl]-.gamma.-oxo-.alpha.,.alpha.-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 149691-84-9 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

RN/ 149691-85-0 HCAPLUS

CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 149691-86-1 HCAPLUS

CN Acetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 149692-10-4 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 149692-11-5 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

RN 149692-12-6 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 149692-13-7 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 149692-14-8 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

CF3

RN 149692-15-9 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-[(phenylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

RN 149692-16-0 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[3-[(methylsulfonyl)amino]-1-oxo-3-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 149692-17-1 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 149692-18-2 HCAPLUS

CN 1-Piperazineacetonitrile, 4-[3-[(aminocarbonyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 149692-20-6 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propenylamino)propyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

RN 149692-21-7 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propynylamino)propyl]- (9CI) (CA INDEX NAME)

RN 149692-24-0 HCAPLUS

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CN 1-Piperazineacetonitrile, 4-[3-[methyl(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

# ●2 HCl

RN 149692-26-2 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl](phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 149692-27-3 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 149692-28-4 HCAPLUS

CN 3-Pyridinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-

# piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 149692-29-5 HCAPLUS CN

Pyrazinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 149692-30-8 HCAPLUS

CN 3-Furancarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

RN 149692-31-9 HCAPLUS

CN 3-Pyridinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-1,2-dihydro-2-oxo-(9CI) (CA INDEX NAME)

PAGE 2-A

RN 149692-41-1 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

RN 150812-47-8 HCAPLUS

CN 1-Piperazineacetonitrile, 4-[4-(3-hydroxy-2-pyridinyl)-1,4-dioxo-3-phenylbutyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 150812-48-9 HCAPLUS

CN 1-Piperazinebutanamide, 4-[cyano(2-methyl-3-pyridinyl)methyl]-N-methyl-.gamma.-oxo-.alpha.-phenyl- (9CI) (CA INDEX NAME)

RN 150812-49-0 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-[(3-pyridinylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 150812-50-3 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propenylamino)propyl]- (9CI) (CA INDEX NAME)

RN 150812-51-4 HCAPLUS

CN 1-Piperazineacetonitrile, 4-[3-[methyl(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

IT 149691-82-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn., deprotection, and platelet aggregation factor antagonistic activity of)

RN 149691-82-7 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 149692-09-1P, UR 12519

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn., platelet aggregation factor antagonistic activity, and toxicity of)

RN 149692-09-1 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, methyl ester (9CI) (CA INDEX NAME)

IT 149691-83-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn., reactions, and platelet aggregation factor antagonistic activity of)

RN 149691-83-8 HCAPLUS

CN 1-Piperazineacetonitrile, 4-(3-amino-1-oxo-3-phenylpropyl)-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

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STRUCTURE FILE UPDATES: 19 MAR 2003 HIGHEST RN 500101-42-8 DICTIONARY FILE UPDATES: 19 MAR 2003 HIGHEST RN 500101-42-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d reg 115 tot 1 RN 357646-20-9 REGISTRY 2 RN 357645-58-0 REGISTRY 3 RN357645-57-9 REGISTRY 4 RN357645-55-7 REGISTRY 5 RN357645-52-4 REGISTRY 6 RN357187-91-8 REGISTRY 7 RN 357187-79-2 REGISTRY 8 RN357187-78-1 REGISTRY

10	RN RN		REGISTRY REGISTRY
11	RN		REGISTRY
$\overline{12}$	RN	260441-62-1	REGISTRY
13	RN -r	260440=99-1	REGISTRY
14	ŖŇ	260440=89-9	REGISTRY
<b>#15</b>	ŔN	260440-84-4	REGĪSTRY
16	RN	* <u>1</u> 260440-57-1.	REGISTRY
17	ŔŊ	260440-23-1	ŖĒĞISTŖY
18 19	RN RN	*260440-19-5 260440-10-6	REGISTRY REGISTRY
20	RN	260440-05-9	REGISTRY
21	RN	260439-80-3	REGISTRY
22	RN	260439=32-5	REGISTRY
23	RN	260439-31-4	REGISTRY
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25	RN	260439-17-6	REGISTRY
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34	RN	161180-96-7	REGISTRY
35	RN	161180-95-6	REGISTRY
36	RN	161180-94-5	REGISTRY
37	RN	150812-51-4	REGISTRY
38	RN	150812 <del>-</del> 50-3	REGISTRY
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40	RN	150812-48-9	REGISTRY
41	RN	150812-47-8	REGISTRY
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45	RN	149692-42-2	REGISTRY
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47	RN	149692-40-0	REGISTRY
48	RN	149692-32-0	REGISTRY
49	RN	149692-31-9	REGISTRY
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53	RN	149692-27-3	REGISTRY
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57	RN	149692-22-8	REGISTRY
58	RN	149692-21-7	REGISTRY
59	RN	149692-20-6	REGISTRY
60	RN	149692-19-3	REGISTRY
61	RN	149692-18-2	REGISTRY
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71	RN	149691-86-1	REGISTRY
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RN

357646-20-9 REGISTRY Piperazine, 1-[[2-(4-chlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]-4-CN (5-chloro-2-pyridinyl) - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 Cl2 N4 O4 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

1: 135:211053 REFERENCE

L15 ANSWER 2 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 357645-58-0 REGISTRY

Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-CN thienyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H19 C1 N4 O4 S2

SR CA

LCSTN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:211053

L15 ANSWER 6 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 357187-91-8 REGISTRY

CN Benzeneacetic acid, .alpha.-[[[4-(5-chloro-2-pyridinyl)-1-

piperazinyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 C1 N3 O4 S

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:195577

L15 ANSWER 10 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 260441-75-6 REGISTRY

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-

(hydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H19 C13 N4 O3 S

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 13 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 260440-99-1 REGISTRY

CN Piperazine, 1-[[2-(5-bromo-3-pyridinyl)-2-(formylhydroxyamino)ethyl]sulfon yl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H19 Br C1 N5 O4 S

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 15 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 260440-84-4 REGISTRY

CN Piperazine, 1-(5-cyano-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H20 N6 O4 S

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 21 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 260439-80-3 REGISTRY

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[(2S)-2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H20 C1 N5 O4 S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 29 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 260438-37-7 REGISTRY

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[[2-(formylhydroxyamino)-2-(2-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C17 H20 C1 N5 O4 S

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 33 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 161180-97-8 REGISTRY

CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C38 H36 N6 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 122:160682

L15 ANSWER 37 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 150812-51-4 REGISTRY

CN 1-Piperazineacetonitrile, 4-[3-[methyl(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C29 H33 N5 O

CI COM

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

L15 ANSWER 42 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-45-5 REGISTRY

CN 1-Piperazineacetonitrile, 4-[3-[[(hydroxymethylamino)carbonyl]amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H28 N6 O3

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 45 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-42-2 REGISTRY

CN Acetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-N-hydroxy- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H27 N5 O3

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 50 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-30-8 REGISTRY

CN 3-Furancarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C26 H27 N5 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 55 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-25-1 REGISTRY

CN 1-Piperazineacetonitrile, 4-[3-[bis(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C35 H37 N5 O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 60 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-19-3 REGISTRY

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-

3-[(2-pyridinylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C27 H30 N6 O

SR CA

LC STN Files: CA, CAPLUS

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 65 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149692-14-8 REGISTRY

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl]-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H26 F3 N5 O3

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

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DATA AVAILABLE IN

2 REFERENCES IN FILE CA (1962 TO DATE) 2 REFERENCES, IN FILE CAPLUS (1962 TO DATE)

REFERENCE 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 71 OF 80 REGISTRY COPYRIGHT 2003 ACS

149691-86-1 REGISTRY RN

CNAcetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl] oxo-1-phenylpropyl] - (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H27 N5 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 77 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 121118-99-8 REGISTRY

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[4-[(4,5dihydroxy-2-pyridinyl)methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]pheny lacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt,

[2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H29 N7 O10 S . Na

SR

LCSTN Files: CA, CAPLUS, TOXCENTER

CRN (121102-21-4)

Absolute stereochemistry.

Na

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092

L15 ANSWER 78 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 121102-36-1 REGISTRY

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[4-[4.5-bis(phenylmethoxy)-2-pyridinyl]methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C49 H47 N7 O10 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

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Ph

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092

L15 ANSWER 80 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 121102-21-4 REGISTRY

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[4-[(4,5-dihydroxy-2-pyridinyl)methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]pheny lacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H29 N7 O10 S

CI COM

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092